PROCESS SIMULATION MODEL FOR INDIRECT COAL LIQUEFACTION USING SLURRY REACTOR FISCHER-TROPSCH TECHNOLOGY

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INTRODUCTION

A detailed baseline design for indirect coal liquefaction using advanced Fischer-Tropsch (F-T) technology has been developed for Illinois No. 6 coal. This design forms the basis for an ASPEN process flowsheet simulation (PFS) model which can simulate the entire liquefaction plant and predict the effects of key process variables on the overall plant performance. A linear programming (LP) model based on a typical PADD II refinery was developed for product valuation and a discounted cash flow (DCF) spreadsheet model was developed for economic analysis. These closely coupled models constitute a research tool which the DOE can use to plan, guide and evaluate its ongoing and future research programs for the manufacture of synthetic liquid fuels by indirect coal liquefaction.

This paper covers the use of the ASPEN process simulation model and DCF spreadsheet model to look at the sensitivity of the economics to certain global process variables such as coal feed rate, synthesis gas conversion per pass and wax yield, together with certain specific reactor operating variables such as temperature, superficial velocity, slurry concentration, catalyst activity and catalyst life. Results are reported in terms of investment cost, yields and operating costs, which are then combined to determine a crude oil equivalent (COE) price. The COE is a hypothetical breakeven crude oil price at which a typical PADD II refinery could buy either crude oil or the coal liquefaction products. It is a present day value and is defined assuming constant deltas between crude oil and its products (i.e. constant refinery processing costs and margins).

OVERALL PLANT DESIGN

Block Flow Diagram

Figure 1 is a block flow diagram showing the overall process configuration. The facility is divided into three main sections:

1. Syngas production. Synthesis gas is generated in Shell gasifiers from ground, dried coal. Processing of the raw synthesis gas from the gasifiers is conventional, with wet scrubbing followed by single stage COS/HCN Hydrolysis and Cooling, Acid Gas Removal by inhibited amine solution and Sulfur Polishing. Sour Water Stripping and Sulfur Recovery units are included in this section.

2. The Fischer-Tropsch synthesis loop. The synthesis loop includes F-T Synthesis, CO_2 Removal, Recycle Gas Compression/Dehydration, Hydrocarbon Recovery by deep refrigeration, Hydrogen Recovery and Autothermal Reforming. The Hydrocarbon Recovery Unit also includes deethanization, depentenization, fractionation and an oxygenates wash column. At low H_2/CO ratios, CO_2 is the primary byproduct of the F-T reaction so a large CO_2 removal unit is required. In the Autothermal Reformer, unrecovered light hydrocarbons in the recycle gas are converted to additional syngas which raises the H_2/CO ratio to the F-T reactors.

3. Product upgrading. The downstream upgrading units include Wax Hydrocracking, Distillate and Naphtha Hydrotreating for oxygenate removal and olefin saturation, Catalytic Naphtha Reforming, C_4 Isomerization, once-through C_5/C_6 Isomerization, $C_3/C_4/C_5$ Alkylation and a Saturate Gas Plant. Liquid wax from the reactor, after catalyst recovery, is sent to the hydrocracker where high quality distillates are produced along with some naphtha and light ends. The naphtha, along with hydrotreated F-T naphtha, is catalytically reformed into aromatic gasoline blending components. Light hydrocarbons are isomerized and alkylated into quality gasoline blending stocks.

The F-T slurry reactor is essentially a bubble column reactor where the slurry phase is a mixture of molten wax and catalyst. The gas provides the agitation necessary for good mixing and mass transfer of reactants to, and products from, the liquid phase. The slurry reactor was chosen over the fixed-bed reactor for the Fischer-Tropsch section based on an earlier Bechtel study[1,2].

Further details concerning the design basis, process selection, cost estimating procedures and alternative cases studied are given in a paper presented at the 1993 DOE/Coal Liquefaction and Gas Conversion Contractors Review Conference[3].

Product and Byproduct Yields

The F-T liquefaction facility produces C_3 LPG, an upgraded C_5 - 350 °F naphtha and 350 °F - 850 °F combined light and heavy distillates. The primary byproduct is liquid sulfur. Yields and product qualities, along with the baseline design F-T reactor operating conditions are given in Table 1. The hydrocarbon products have no measurable sulfur or nitrogen contents because of the requirements and nature of the Fischer-Tropsch reaction. Oxygen is removed to less than 30 ppmv. There are virtually no aromatics in the distillate. Olefins are saturated to low levels of residual olefin concentration in both the naphtha and the distillate. The diesel fraction has a very high cetane number, on the order of 70, and the jet fuel fraction and heavy distillates have low smoke points.

The naphtha product is a mixture of $C_3/C_4/C_5$ alkylate, C_5/C_6 isomerate and catalytic reformate. It is basically a raw gasoline with a clear (R+M)/2 octane number of about 88. If insufficient butanes are available to alkylate all of the available C3/C4/C5 olefins, then n-butane is purchased and isomerized.

PROCESS SIMULATION MODEL

The process flowsheet simulation model predicts the effects of key process variables on the overall material and utility balances, operating requirements and capital costs. This model is implemented in the PC version of ASPEN/SP.

Development of the Model

Baseline design information was transmitted from Bechtel to Amoco for the development of the process flowsheet simulation computer model. Information transfer was expedited by Bechtel's development of a preliminary ASPEN/SP model for the design of the F-T synthesis loop. The computerized F-T slurry reactor yield correlations used for design purposes have been discussed previously[4].

The computer model was developed as a planning/research guidance tool for the DOE and its subcontractors. The model is not designed to be a plant design and sizing program for every plant in the complex. The F-T synthesis loop design is handled in some detail and Bechtel's F-T reactor sizing and yield models are built into the design. For other plants, only overall yield, utility requirements and capital costs are estimated. Costs are prorated on capacity using cost-capacity exponents and information on the maximum and minimum capacity of single train plants.

All ISBL plants in the three main processing sections discussed earlier are simulated; some by a combination of ASPEN/SP process simulation blocks and user Fortran blocks and some by just user Fortran blocks. Material balances, as well as utility consumptions, operating personnel requirements and ISBL costs for each plant are produced. The OSBL, engineering and contingency costs are estimated from the ISBL plant costs to generate the total installed cost of the facility.

This ASPEN model generates a file for direct transfer of the significant model results to the DCF spreadsheet economics model. The spreadsheet model takes this input, and with a given set of financial assumptions calculates the cost of production and a crude oil equivalent price for a 15% return on investment.

F-T product values were generated by a linear programming model of a typical PADD II refinery at present day crude oil prices. These results are being reported separately at this meeting[5]. In calculating the COE, several different assumptions can be used to relate feed and product values to crude oil price. The DCF spreadsheet allows for the use of a constant value, a constant ratio or a constant delta. Since what is desired is the equivalent refinery processing cost to produce the same product, this paper uses a constant delta to relate the hydrocarbon products and imported butane prices to the crude oil price. The effect of varying these deltas is shown.

Caution should be used in extrapolating COE to future pricing scenarios and drawing conclusions as to when coal liquids will become competitive with equivalent products from crude oil. The COE, as herein defined, is a conceptual tool allowing various yield configurations and coal processing scenarios to be compared as a single number on the basis of present day economics. When future projections are made, it is necessary to consider inflation in construction costs as well as various price escalation scenarios for crude oil, coal and other energy sources. Such studies are beyond the scope of this paper.

PROCESS SENSITIVITY STUDIES

The PFS model is designed to handle the effects of the following process variables:

Primary Variables	Range
Coal Feed Rate	4,500 to 45,000 mtpd
F-T Conversion per Pass	50 to 82%
F-T Wax Yield	10 to 75%
F-T Reactor Inlet Superficial Velocity	5 to 20 cm/s
F-T Reactor Catalyst Concentration	20 to 40%
Secondary Variables	
H_2/CO Ratio	0.36 to 0.7
Heat Transfer Flux	68,000 KJ/hr-m^2 - 114,000 KJ/hr-m^2 (6,000 - 10,000 Btu/hr-ft^2)
Flow Regime	Bubble to Churn Turbulent

Baseline design conditions are 18,400 mtpd coal feed rate, 82% conversion, 50% wax yield, 10 cm/s superficial velocity and 22.5 wt% slurry.

This paper presents the results of parametric economic studies covering the primary variables cited above. A brief summary follows:

Effect of Design Plant Capacity - The effect of plant capacity on the overall F-T facility capital investment is exponential with an average cost-capacity exponent of 0.89..This large an exponent is not surprising since multiple process trains are involved. The effect on COE, over the entire range, is about $0.80/bbl.

Effect of Design F-T Syngas Conversion Per Pass - As expected, high conversion per pass is economically favorable. Decreasing the syngas conversion from 82 to 68% at a constant 18,400 mtpd coal feed rate increases total plant investment by approximately 9%, with the main effect being on the F-T synthesis section loop due to increased recycle. The L/D of the F-T reactor becomes much smaller at low conversion and the designs become impractical unless other parameters, such as slurry concentration, are relaxed as well.

Effect of Design Wax Yield - The effect of design wax yield at the baseline capacity of 18,400 mtpd coal feed rate was studied over the range of 10 to 75 wt%, obtained by varying F-T reactor temperature from 271 to 242 °C. Increasing the wax yield from 10 to 75 wt% reduces the F-T naphtha to distillates production ratio from 2.38 to 0.62. An increase in light olefins production at 10 wt% wax yield requires the purchase of roughly 11,000 bbl/day of butane to make alkylate, whereas the 75 wt% wax yield case is in butane balance.

The F-T reactor size becomes larger at high wax yield and there is a minimum in plant investment cost at about 50 wt% wax yield. The variation in total plant cost, over the entire range of wax yields, is less than 3%. The optimum wax yield is highly dependent on the price of purchased butane, gasoline and diesel relative to crude oil. Present day price spreads for F-T gasoline and distillates relative to crude oil were determined as $9.00/bbl and $6.90/bbl, respectively, by linear programming studies[5]. The present price for butane is $3.50/bbl. less than crude oil. Using these deltas, the optimum wax yield appears to fall between 50 to 60 wt%.

Lowering the butanes price relative to crude oil drastically alters this trend, and when butanes are priced at $20/bbl under the price of crude oil, the low wax yield case is preferred. The linear programming studies did not credit the exceptionally high cetane number of the F-T distillate product. Other sources indicate that a delta of $9.0/bbl instead of $6.90/bbl for the F-T distillates may be more realistic and this lowers the COE by $1.00 per barrel and makes the optimum wax yield slightly higher.

Effect of Slurry F-T Reactor Design Variables - The inlet superficial gas velocity was studied in conjunction with slurry concentration. The reason is that, if varied independently, as soon as these variable depart from the baseline design, the reactor L/D changes. Increasing superficial velocity, at constant slurry concentration, leads to impractically high L/D ratios for which the costing algorithm is not equipped to handle accurately. This can be compensated for by increasing slurry concentration. Figure 2 shows the combination of superficial velocity and slurry concentration necessary to maintain a constant L/D of 3.15 (the baseline design reactor). The reactor inside diameter has been kept between 3.8 to 5.0 meters (12.5 to 16.5

feet) by varying the number of reactors from 48 to 16. The baseline design, at 10cm/s superficial velocity and 22.5 wt% slurry concentration, has eight F-T synthesis trains with 3 reactors per train, each reactor being 5 meters ID by 15.8 meters T-T.

Figure 2 also shows the total cost of reactors as a function of the superficial velocity and slurry concentration while maintaining a constant reactor L/D of 3.15. The cost is inversely proportional to the inlet superficial gas velocity. The potential savings on increasing the superficial gas velocity from 5 to 20 cm/s is on the order of $80 million, and this results in a reduction of the COE by about $0.80/bbl.

CONCLUSIONS AND RECOMMENDATIONS

These preliminary parametric sensitivity studies demonstrate the capability of the process flowsheet simulation model. When coupled to a discounted cash flow spreadsheet model, its effectiveness for examining the effects of various process variables on the F-T indirect coal liquefaction costs and economics has been demonstrated. The responsiveness of the model to a variety of F-T slurry reactor operating conditions has also been established.

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<u>Table 1</u>
Baseline Facility Design

<u>Feed:</u>	
ROM as received coal	7.68×10^5 Kg/hr (18,420 mtpd)
N-Butane	1.20×10^4 Kg/hr (3,120 BPSD)
Electric power	50 MWh
<u>Primary Products:</u>	
C3 LPG	6.45×10^3 Kg/hr (1,920 BPSD)
F-T gasoline blend	1.14×10^5 Kg/hr (23,900 BPSD)
F-T diesel blend	1.26×10^5 Kg/hr (24,700 BPSD)
Sulfur	2.12×10^4 Kg/hr
<u>F-T Operating Conditions:</u>	
Temperature/pressure	253 °C/2.17 MPa (50% wax)
Syngas conversion	81.7 %
Inlet superficial gas velocity	10.0 cm/sec
Catalyst slurry concentration	22.5 wt%
Catalyst make-up rate	0.5 % per day

mtpd [=] metric tons per stream day
BPSD [=] Barrels per stream day

Figure 1
INDIRECT COAL LIQUEFACTION BASELINE STUDY
OVERALL PROCESS CONFIGURATION

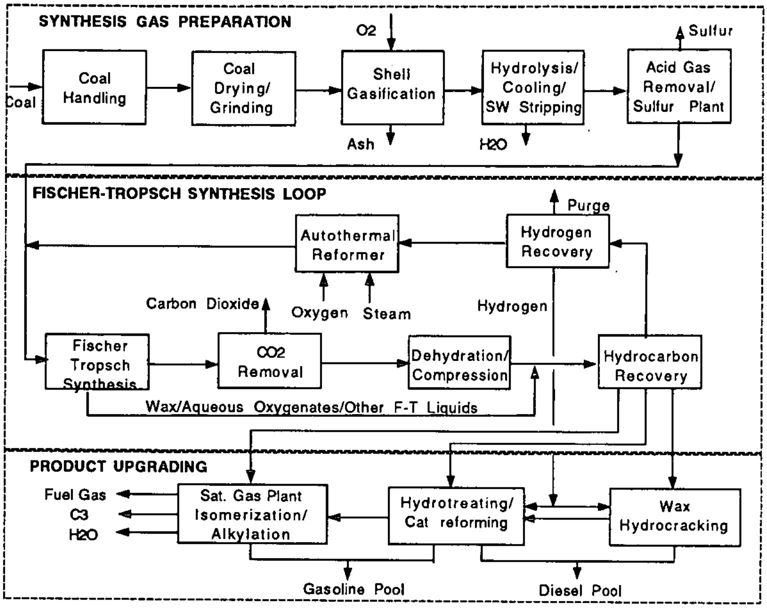

Figure 2
Total F-T Reactor Cost at Constant L/D of 3.15